

4-Methylbenzenesulfonic acid  
104-15-4 | DTXSID0026701

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

## Model Results

**Predicted value:** 5.74

**Global applicability domain:** Inside

**Local applicability domain index:** 3.76e-01

**Confidence level:** 7.96e-01

## Nearest Neighbors from the Training Set

Image not found

Sodium 3-nitrobenzenesulfonate

**Measured:** 5.01

**Predicted:** 5.24

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Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt

**Measured:** 3.02

**Predicted:** 5.14

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4-Hydroxy-1-naphthalenesulfonic acid monosodium salt

**Measured:** 12.9

**Predicted:** 6.33

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Phenylphosphinic acid

**Measured:** 6.03

**Predicted:** 4.42

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4-Amino-1-naphthalenesulfonic acid sodium salt

**Measured:** 6.03

**Predicted:** 5.38